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Algorithm for Generating Quasiperiodic Packings of Multi-Shell Clusters

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Abstract

Many of the mathematical models used in quasicrystal physics are based on tilings of the plane or space obtained by using strip projection method in a superspace of dimension four, five or six. We present some mathematical results which allow one to use this very elegant method in spaces of dimension much higher and to generate directly quasiperiodic packings of multi-shell clusters. We show that in the case of a two-dimensional (resp. three-dimensional) cluster we have to compute only determinants of order three (resp. four), independently of the dimension of the superspace we use. The computer program based on our mathematical results is very efficient. For example, we can easily generate quasiperiodic packings of three-shell icosahedral clusters (icosahedron + dodecahedron + icosidodecahedron) by using strip projection method in a 31-dimensional space (hundreds of points are obtained in a few minutes on a personal computer).

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Quasicrystals are materials with perfect long-range order, but with no three-dimensional translational periodicity. The discovery of these solids [1] in the early 1980's and the challenge to describe their structure led to a great interest in quasiperiodic sets of points. The diffraction image of a quasicrystal often contains a set of sharp Bragg peaks invariant under a finite non-crystallographic group of symmetries G, called the symmetry group of quasicrystal (in reciprocal space). In the case of quasicrystals with no translational periodicity this group is the icosahedral group Y and in the case of quasicrystals periodic along one direction (two-dimensional quasicrystals) G is one of the dihedral groups D_8 (octagonal quasicrystals), D_{10} (decagonal quasicrystals) and D_{12} (dodecagonal quasicrystals).

Real structure information obtained by high resolution transmission electron microscopy suggests us that a quasicrystal with symmetry group G can be regarded as a quasiperiodic packing of interpenetrating (partially occupied) copies of a well-defined G-invariant cluster $\mathcal{C}$. From a mathematical point of view, a G-cluster is a finite union of orbits of G in a fixed representation of G. A mathematical algorithm for generating quasiperiodic packings of interpenetrating copies of G-clusters was proposed by author in collaboration with Jean-Louis Verger-Gaugry several years ago [2, 3]. This algorithm based on strip projection method has been considered difficult to use since the dimension of the involved superspace is rather high. The mathematical results we present in the present paper simplifies the computer program and allow to use strip projection method in superspaces of large dimension.

The dihedral group D_{2m} can be defined in terms of generators and relations as

$$D_{2m} = \langle\ a,\ b\ |\ \ a^{2m} = b^2 = (ab)^2 = e\ \rangle \tag{1}$$

and the relations

$$a(\alpha,\beta) = \left(\alpha\,\cos\frac{\pi}{m} - \beta\,\sin\frac{\pi}{m},\ \alpha\,\sin\frac{\pi}{m} + \beta\,\cos\frac{\pi}{m}\right) \qquad b(\alpha,\beta) = (\alpha,-\beta) \tag{2}$$

define an $\mathbb{R}$-irreducible representation in $\mathbb{R}^2$. The orbit of D_{2m} generated by $(\alpha,\beta)\in\mathbb{R}^2$

$$D_{2m}(\alpha,\beta) = \{\ g(\alpha,\beta)\ |\ g\in D_{2m}\ \} = \{(\alpha,\beta), a(\alpha,\beta),\ a^2(\alpha,\beta),\ ...,\ a^{2m-1}(\alpha,\beta)\} \tag{3}$$

contains $2m$ points (vertices of a regular polygon with $2m$ sides). A two-shell D_{2m}-cluster $\mathcal{C}_2$ is a union of two orbits $\mathcal{C}_2 = D_{2m}(\alpha_1,\beta_1)\cup D_{2m}(\alpha_2,\beta_2)$.

The icosahedral group $Y = 235$ can be defined in terms of generators and relations as

$$Y = \langle a, b\ |\ a^5 = b^2 = (ab)^3 = e\rangle \tag{4}$$

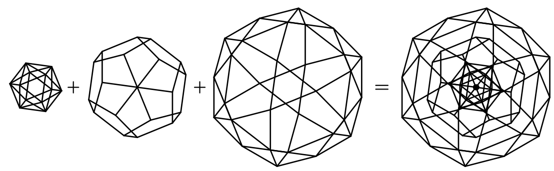

FIG. 1: A three-shell icosahedral cluster is a union of three orbits of Y.

and the rotations $a,\, b:\mathbb{R}^3 \longrightarrow \mathbb{R}^3$

$$\begin{aligned} a(\alpha,\beta,\gamma) &= \left(\tfrac{\tau-1}{2}\alpha - \tfrac{\tau}{2}\beta + \tfrac{1}{2}\gamma,\ \tfrac{\tau}{2}\alpha + \tfrac{1}{2}\beta + \tfrac{\tau-1}{2}\gamma,\ -\tfrac{1}{2}\alpha + \tfrac{\tau-1}{2}\beta + \tfrac{\tau}{2}\gamma\right) \\ b(\alpha,\beta,\gamma) &= (-\alpha,-\beta,\gamma). \end{aligned} \tag{5}$$

where $\tau = (1+\sqrt{5})/2$, generate an irreducible representation of Y in $\mathbb{R}^3$. In the case of this representation there are the trivial orbit $Y(0,0,0) = \{(0,0,0)\}$ of length 1, the orbits

$$Y(\alpha,\alpha\tau,0) = \{g(\alpha,\alpha\tau,0)\ |\ g \in Y\} \qquad \text{where} \quad \alpha \in (0,\infty) \tag{6}$$

of length 12 (vertices of a regular icosahedron), the orbits

$$Y(\alpha,\alpha,\alpha) = \{g(\alpha,\alpha,\alpha)\ |\ g \in Y\} \qquad \text{where} \quad \alpha \in (0,\infty) \tag{7}$$

of length 20 (vertices of a regular dodecahedron), the orbits

$$Y(\alpha,0,0) = \{g(\alpha,0,0)\ |\ g \in Y\} \qquad \text{where} \quad \alpha \in (0,\infty) \tag{8}$$

of length 30 (vertices of an icosidodecahedron), and all the other orbits are of length 60. The union of orbits $\mathcal{C}_3 = Y(\alpha,\alpha\tau,0) \cup Y(\beta,\beta,\beta) \cup Y(\gamma,0,0)\}$ is a three-shell icosahedral cluster (Fig. 1).

In order to have explicit mathematical formulae, we start by presenting our results in a particular case, namely, $G = D_{10}$. Let

$$\mathcal{C}_2 = D_{10}(\alpha_1,\beta_1) \cup D_{10}(\alpha_2,\beta_2) = \{v_1,\ v_2,\ ...,\ v_{10},\ -v_1,\ -v_2,\ ...,\ -v_{10}\} \tag{9}$$

where

$$v_1 = (v_{11}, v_{21}), \quad v_2 = (v_{12}, v_{22}), \quad ..., \quad v_{10} = (v_{1\,10}, v_{2\,10}) \tag{10}$$

be a fixed two-shell D_{10}-cluster, and let

$$w_1 = (v_{11}, v_{12}, ..., v_{1\,10}) \qquad \text{and} \qquad w_2 = (v_{21}, v_{22}, ..., v_{2\,10}). \tag{11}$$

From the general theory [2, 3] (a direct verification is also possible) it follows that the vectors w_1 and w_2 from $\mathbb{R}^{10}$ have the same norm and are orthogonal

$$\begin{array}{l} v_{11}^2 + v_{12}^2 + ... + v_{1\,10}^2 = v_{21}^2 + v_{22}^2 + ... + v_{2\,10}^2 \\ \langle w_1, w_2 \rangle = v_{11}v_{21} + v_{12}v_{22} + ... + v_{1\,10}v_{2\,10} = 0. \end{array} \tag{12}$$

We identify the physical space with the two-dimensional subspace

$$\boldsymbol{E}_2 = \{ \ \alpha w_1 + \beta w_2 \mid \alpha, \ \beta \in \mathbb{R} \ \} \tag{13}$$

of the superspace $\mathbb{R}^{10}$ and denote by $\boldsymbol{E}_2^{\perp}$ the orthogonal complement

$$\boldsymbol{E}_2^{\perp} = \{ \ x \in \mathbb{R}^{10} \mid \langle x, y \rangle = 0 \text{ for all } y \in \boldsymbol{E}_2 \ \}. \tag{14}$$

The orthogonal projection onto $\boldsymbol{E}_2$ of a vector $x \in \mathbb{R}^{10}$ is the vector

$$\pi\, x = \left\langle x, \frac{w_1}{\kappa} \right\rangle \frac{w_1}{\kappa} + \left\langle x, \frac{w_2}{\kappa} \right\rangle \frac{w_2}{\kappa} \tag{15}$$

where $\kappa = ||w_1|| = ||w_2||$, and the orthogonal projector corresponding to $\boldsymbol{E}_2^{\perp}$ is

$$\pi^{\perp} : \mathbb{R}^{10} \longrightarrow \boldsymbol{E}_2^{\perp} \qquad \pi^{\perp} x = x - \pi\, x. \tag{16}$$

If we describe $\boldsymbol{E}_2$ by using the orthogonal basis $\{\kappa^{-2} w_1, \ \kappa^{-2} w_2\}$ then the orthogonal projector corresponding to $\boldsymbol{E}_2$ is

$$\mathcal{P}_2 : \mathbb{R}^{10} \longrightarrow \mathbb{R}^2 \qquad \mathcal{P}_2 x = (\langle x, w_1 \rangle, \langle x, w_2 \rangle). \tag{17}$$

The projection $\boldsymbol{W}_{2,10} = \pi^{\perp}(\boldsymbol{\Omega}_{10})$ of the unit hypercube

$$\boldsymbol{\Omega}_{10} = [-0.5, \ 0.5]^{10} = \{(x_1, x_2, ..., x_{10}) \mid \ -0.5 \leq x_i \leq 0.5 \text{ for all } i \in \{1, 2, ..., 10\} \ \}. \tag{18}$$

is a polyhedron (called the *window* of selecton) in the 8-dimensional subspace $\boldsymbol{E}_2^{\perp}$, and each 7-dimensional face of $\boldsymbol{W}_{2,10}$ is the projection of a 7-dimensional face of $\boldsymbol{\Omega}_{10}$. The vectors

$$\begin{array}{rcl} e_1 & = & (1,0,0,0,0,0,0,0,0,0) \\ e_2 & = & (0,1,0,0,0,0,0,0,0,0) \\ ... & ... & .... \\ e_{10} & = & (0,0,0,0,0,0,0,0,0,1) \end{array} \tag{19}$$

form the canonical basis of $\mathbb{R}^{10}$, and each 7-face of $\mathbf{\Omega}_{10}$ is parallel to seven of these vectors and orthogonal to three of them. There exist eight 7-faces of $\mathbf{\Omega}_{10}$ orthogonal to the distinct vectors e_{i_1}, e_{i_2}, e_{i_3}, and the set

$$\left\{ x = (x_1, x_2, ..., x_{10}) \;\middle|\; \begin{array}{ll} x_i \in \{-0.5,\, 0.5\} & \text{if } i \in \{i_1,\, i_2,\, i_3\} \\ x_i = 0 & \text{if } i \notin \{i_1,\, i_2,\, i_3\} \end{array} \right\} \tag{20}$$

contains one and only one point from each of them. There are

$$\begin{pmatrix} 10 \\ 3 \end{pmatrix} = \frac{10 \cdot 9 \cdot 8}{1 \cdot 2 \cdot 3} = 210 \tag{21}$$

sets of 8 parallel 7-faces of $\mathbf{\Omega}_{10}$, and we label them by using the elements of the set

$$\mathcal{I}_{2,10} = \{(i_1, i_2, i_3) \in \mathbb{Z}^3 \mid 1 \leq i_1 \leq 8, \quad i_1 + 1 \leq i_2 \leq 9, \quad i_2 + 1 \leq i_3 \leq 10 \;\}. \tag{22}$$

In $\mathbb{R}^3$ the cross-product of two vectors $\boldsymbol{v} = (v_x, v_y, v_z)$ and $\boldsymbol{w} = (w_x, w_y, w_z)$ is a vector orthogonal to $\boldsymbol{v}$ and $\boldsymbol{w}$, and can be obtained by expanding the formal determinant

$$\boldsymbol{v} \times \boldsymbol{w} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{vmatrix} \tag{23}$$

where $\{\boldsymbol{i},\, \boldsymbol{j},\, \boldsymbol{k}\}$ is the canonical basis of $\mathbb{R}^3$. For any vector $\boldsymbol{u} = (u_x, u_y, u_z)$, the scalar product of $\boldsymbol{u}$ and $\boldsymbol{v} \times \boldsymbol{w}$ is

$$\boldsymbol{u}(\boldsymbol{v} \times \boldsymbol{w}) = \begin{vmatrix} u_x & u_y & u_z \\ v_x & v_y & v_z \\ w_x & w_y & w_z \end{vmatrix}. \tag{24}$$

In a very similar way, a vector y orthogonal to nine vectors

$$u_i = (u_{i1}, u_{i2}, u_{i3}, ..., u_{i\,10}) \qquad i \in \{1, 2, 3, ..., 9\} \tag{25}$$

from $\mathbb{R}^{10}$ can be obtained by expanding the formal determinant

$$y = \begin{vmatrix} e_1 & e_2 & e_3 & ... & e_{10} \\ u_{11} & u_{12} & u_{13} & ... & u_{1\,10} \\ u_{21} & u_{22} & u_{23} & ... & u_{2\,10} \\ ... & ... & ... & ... & ... \\ u_{91} & u_{92} & u_{93} & ... & u_{9\,10} \end{vmatrix} \tag{26}$$

containing the vectors of the canonical basis in the first row. For any $x \in \mathbb{R}^{10}$, the scalar product of x and y is

$$\langle x, y \rangle = \begin{vmatrix} x_1 & x_2 & x_3 & ... & x_{10} \\ u_{11} & u_{12} & u_{13} & ... & u_{1\,10} \\ u_{21} & u_{22} & u_{23} & ... & u_{2\,10} \\ ... & ... & ... & ... & ... \\ u_{91} & u_{92} & u_{93} & ... & u_{9\,10} \end{vmatrix} . \tag{27}$$

For example,

$$y = \begin{vmatrix} e_1 & e_2 & e_3 & e_4 & e_5 & e_6 & e_7 & e_8 & e_9 & e_{10} \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ v_{11} & v_{12} & v_{13} & v_{14} & v_{15} & v_{16} & v_{17} & v_{18} & v_{19} & v_{1\,10} \\ v_{21} & v_{22} & v_{23} & v_{24} & v_{25} & v_{26} & v_{27} & v_{28} & v_{29} & v_{2\,10} \end{vmatrix} = \begin{vmatrix} e_1 & e_2 & e_3 \\ v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{vmatrix} \tag{28}$$

is a vector orthogonal to the vectors e_4, e_5, ..., e_{10}, w_1, w_2, and

$$\langle x, y \rangle = \begin{vmatrix} x_1 & x_2 & x_3 \\ v_{11} & v_{12} & v_{13} \\ v_{21} & v_{22} & v_{23} \end{vmatrix} \tag{29}$$

for any $x \in \mathbb{R}^{10}$. The vector y belongs to $\boldsymbol{E}_2^{\perp}$, and since $e_i - \pi^{\perp} e_i$ is a linear combination of w_1 and w_2, it is also orthogonal to $\pi^{\perp} e_4$, $\pi^{\perp} e_5$, ..., $\pi^{\perp} e_{10}$. Therefore, y is orthogonal to the 7-faces of $\boldsymbol{W}_{2,10}$ labelled by $(1, 2, 3)$. Similar results can be obtained for any $(i_1, i_2, i_3) \in \mathcal{I}_{2,10}$.

Consider the *strip* corresponding to $\boldsymbol{W}_{2,10}$ (Fig. 2)

$$\boldsymbol{S}_{2,10} = \{ x \in \mathbb{R}^{10} \mid \pi^{\perp} x \in \boldsymbol{W}_{2,10} \} \tag{30}$$

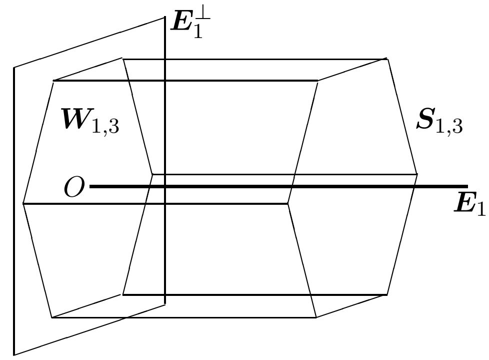

FIG. 2: The window $\boldsymbol{W}_{1,3}$ and the corresponding strip $\boldsymbol{S}_{1,3}$ (case of a one-dimensional physical space $\boldsymbol{E}_1$ embedded into a three-dimensional superspace).

and define

$$d_{i_1i_2i_3} = \max_{\alpha_j\in\{0.5,\,0.5\}} \begin{vmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ v_{1i_1} & v_{1i_2} & v_{1i_3} \\ v_{2i_1} & v_{2i_2} & v_{2i_3} \end{vmatrix} \qquad \text{for each} \quad (i_1,i_2,i_3)\in\mathcal{I}_{2,10}. \tag{31}$$

A point $x=(x_1,x_2,...,x_{10})\in\mathbb{R}^{10}$ belongs to the strip $\boldsymbol{S}_{2,10}$ if and only if

$$-d_{i_1i_2i_3} \leq \begin{vmatrix} x_{i_1} & x_{i_2} & x_{i_3} \\ v_{1i_1} & v_{1i_2} & v_{1i_3} \\ v_{2i_1} & v_{2i_2} & v_{2i_3} \end{vmatrix} \leq d_{i_1i_2i_3} \qquad \text{for any} \quad (i_1,i_2,i_3)\in\mathcal{I}_{2,10}. \tag{32}$$

The set defined in terms of the strip projection method [4, 5, 6, 7, 8]

$$\mathcal{Q}_2 = \mathcal{P}_2(\boldsymbol{S}_{2,10}\cap\mathbb{Z}^{10}) = \{\ \mathcal{P}_2 x \ |\ \ x\in\boldsymbol{S}_{2,10}\cap\mathbb{Z}^{10}\ \} \tag{33}$$

can be regarded (Fig. 3) as a quasiperiodic packing of translated (partially occupied) copies of $\mathcal{C}_2$. Since

$$\mathcal{P}_2 e_i = (\langle e_i,w_1\rangle,\langle e_i,w_2\rangle) = (v_{1i},v_{2i}) = v_i \qquad \text{for any } i\in\{1,2,...,10\} \tag{34}$$

we get

$$\begin{aligned} &\mathcal{P}_2\ \ (\{\ \ x\pm e_1,\ x\pm e_2,\ ...,\ x\pm e_{10}\}\cap\boldsymbol{S}_{2,10}) \\ &\qquad \subseteq\ \{\mathcal{P}_2 x\pm v_1,\ \mathcal{P}_2 x\pm v_2\ ...,\ \mathcal{P}_2 x\pm v_{10}\} = \mathcal{P}_2 x+\mathcal{C}_2 \end{aligned} \tag{35}$$

that is, the neighbours of any point $\mathcal{P}_2 x\in\mathcal{Q}_2$ belong to the translated copy $\mathcal{P}_2 x+\mathcal{C}_2$ of $\mathcal{C}_2$.

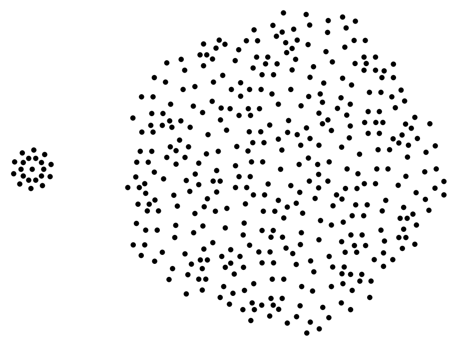

FIG. 3: The two-shell decagonal cluster $\mathcal{C}_2$ and a fragment of $\mathcal{Q}_2$.

Our algorithm works for any finite group G, any $\mathbb{R}$-irreducible representation of G in a space $\mathbb{R}^n$ and any G-cluster symmetric with respect to the origin

$$\mathcal{C}_n = \{v_1,\ v_2,\ ...,\ v_k,\ -v_1,\ -v_2,\ ...,\ -v_k\} \subset \mathbb{R}^n. \tag{36}$$

We identify the 'physical space' with the n-dimensional subspace

$$\boldsymbol{E}_n = \{\alpha_1 w_1 + \alpha_2 w_2 + ... + \alpha_n w_n \mid \alpha_1,\ \alpha_2,\ ...,\ \alpha_n \in \mathbb{R}\ \} \tag{37}$$

of the superspace $\mathbb{R}^k$ spanned by the orthogonal vectors with the same norm

$$w_i = (v_{i1},\ v_{i2},\ ...,\ v_{ik}) \qquad i \in \{1, 2, ..., n\} \tag{38}$$

defined by using the coordinates v_{ij} of the vectors $v_j = (v_{1j}, v_{2j}, ..., v_{nj})$.

The window $\boldsymbol{W}_{n,k} = \pi^\perp(\boldsymbol{\Omega}_k)$ is a polyhedron in the $(k-n)$-subspace $\boldsymbol{E}_n^\perp$. Each $(k-n-1)$-face of $\boldsymbol{W}_{n,k}$ is the projection of a $(k-n-1)$-face of the unit hypercube $\boldsymbol{\Omega}_k = [-0.5,\ 0.5]^k$. Each $(k-n-1)$-face of $\boldsymbol{\Omega}_k$ is parallel to $k-n-1$ vectors of the canonical basis $\{e_1,\ e_2,\ ...,\ e_k\}$ and orthogonal to $n+1$ of them. For each $n+1$ distinct vectors $e_{i_1},\ e_{i_2},\ ...,\ e_{i_{n+1}}$ the number of $(k-n-1)$-faces of $\boldsymbol{\Omega}_k$ orthogonal to them is 2^{n+1}. There are $k!/[(n+1)!\,(k-n-1)!]$ sets of 2^{n+1} parallel $(k-n-1)$-faces of $\boldsymbol{\Omega}_k$. In the case $n=2$ these sets are labelled by

$$\mathcal{I}_{2,k} = \{(i_1, i_2, i_3) \in \mathbb{Z}^3 \mid 1 \le i_1 \le k-2,\quad i_1+1 \le i_2 \le k-1,\quad i_2+1 \le i_3 \le k\ \} \tag{39}$$

and in the case $n=3$ are labelled by

$$\mathcal{I}_{3,k} = \left\{ (i_1, i_2, i_3, i_4) \in \mathbb{Z}^4 \;\middle|\; \begin{array}{r} 1 \le i_1 \le k-3, \quad i_1+1 \le i_2 \le k-2, \\ i_2+1 \le i_3 \le k-1, \quad i_3+1 \le i_4 \le k \end{array} \right\}. \tag{40}$$

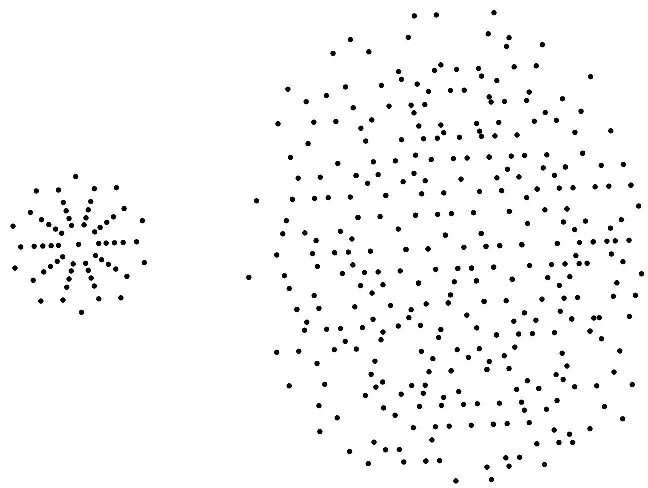

FIG. 4: Projected positions of points of $\mathcal{C}_3$ and of $\mathcal{Q}_3$ down a fivefold axis in the case of an icosahedral three-shell cluster.

In the case $n = 3$, a point $x = (x_1, x_2, ..., x_k) \in \mathbb{R}^k$ belongs to the strip $\boldsymbol{S}_{3,k}$ if and only if

$$-d_{i_1 i_2 i_3 i_4} \leq \left| \begin{array}{cccc} x_{i_1} & x_{i_2} & x_{i_3} & x_{i_4} \\ v_{1i_1} & v_{1i_2} & v_{1i_3} & v_{1i_4} \\ v_{2i_1} & v_{2i_2} & v_{2i_3} & v_{2i_4} \\ v_{3i_1} & v_{3i_2} & v_{3i_3} & v_{3i_4} \end{array} \right| \leq d_{i_1 i_2 i_3 i_4} \qquad \text{for each } (i_1, i_2, i_3 i_4) \in \mathcal{I}_{3,k} \tag{41}$$

where

$$d_{i_1 i_2 i_3 i_4} = \max_{\alpha_j \in \{0.5,\, 0.5\}} \left| \begin{array}{cccc} \alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\ v_{1i_1} & v_{1i_2} & v_{1i_3} & v_{1i_4} \\ v_{2i_1} & v_{2i_2} & v_{2i_3} & v_{2i_4} \\ v_{3i_1} & v_{3i_2} & v_{3i_3} & v_{3i_4} \end{array} \right| . \tag{42}$$

The pattern defined in terms of the strip projection method

$$\mathcal{Q}_n = \mathcal{P}_n(\boldsymbol{S}_{n,k} \cap \mathbb{Z}^k) = \{\mathcal{P}_n x \mid \ x \in \boldsymbol{S}_{n,k} \cap \mathbb{Z}^k \ \} \tag{43}$$

where

$$\mathcal{P}_n : \mathbb{R}^k \longrightarrow \mathbb{R}^n \qquad \mathcal{P}_n x = (\langle x, w_1 \rangle, \langle x, w_2 \rangle, ..., \langle x, w_n \rangle), \tag{44}$$

can be regarded as a quasiperiodic packing of copies of the starting cluster $\mathcal{C}_n$.

Projected positions down a fivefold axis of points of a fragment of the pattern $\mathcal{Q}_3$ obtained by starting from the icosahedral three-shell cluster

$$\mathcal{C}_3 = Y\left(\frac{1}{\sqrt{2+\tau}}, \frac{\tau}{\sqrt{2+\tau}}, 0\right) \cup Y\left(\frac{2}{\sqrt{3}}, \frac{2}{\sqrt{3}}, \frac{2}{\sqrt{3}}\right) \cup Y(3,0,0) \tag{45}$$

are presented in Fig. 4. The dimension k of the superspace in this case is 31.

The description of the atomic structure of quasicrystals is a very difficult problem. Elser & Henley [9] and Audier & Guyot [10] have obtained models for icosahedral quasicrystals by decorating the Ammann rhombohedra occuring in a tiling of the 3D space defined by projection. In his quasi-unit cell picture Steinhardt [11] has shown that the atomic structure can be described entirely by using a single repeating cluster which overlaps (shares atoms with) neighbour clusters. The model is determined by the overlap rules and the atom decoration of the unit cell. Some important models have been obtained by Yamamoto & Hiraga [12, 13], Katz & Gratias [14], Gratias Puyraimond and Quiquandon [15] by using the section method in a six-dimensional superspace decorated with several polyhedra (acceptance domains). Janot and de Boissieu [16] have shown that a model of icosahedral quasicrystal can be generated recursively by starting from a pseudo-Mackay cluster and using some inflation rules. In the case of all these models one has to add or shift some points in order to fill the gaps between the clusters, and one has to elliminate some points from interpenetrating clusters if they become too close.

The strip projection method has been used (to our knowlege) mainly for generating tilings of plane or space, and only in superspaces of dimension four, five or six. Algorithms and details concerning computer programs for generating quasiperiodic tilings have been presented by Conway and Knowles [7], Vogg and Ryder [17],Lord, Ramakrishnan and Ranganathan [18]. We present an algorithm for generating quasiperiodic packings of multi-shell clusters based on strip projection method used in a superspace of large dimension. The quasiperiodic sets obtained in this way have the remarkable mathematical properties of the patterns obtained by projection and the desired local structure. Each point of the set is the centre of a more or less occupied copy of the starting cluster, and the clusters corresponding to neighbouring points share several points. Computer programs in FORTRAN 90 are available via

internet [19].

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